# Lefschetz-thimble & complex Langevin approach to Silver Blaze of one-site Hubbard model

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# Finite-density QCD?

## Neutron star

- Cold and dense nuclear matters
- $2m_{\mathrm{sun}}$ neutron star (2010)
- Gravitational-wave observations (2017$\sim$)

Reliable theoretical approach to equation of state must be developed!

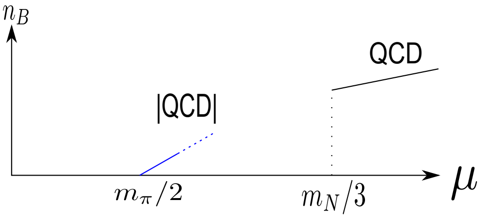
$$Z(T,\mu)=\int \mathcal{D}A\, \underbrace{\mathrm{Det}(\not{D}(A,\mu)+m)}_{\text{quark}}\underbrace{\exp -S_{\mathrm{YM}}(A)}_{\text{gluon}}.$$

# Silver Blaze problem in finite-density QCD

QCD & |QCD|

$$Z_{\mathrm{QCD}}=\int\mathcal{D}A\,(\det\gamma_\nu D_\nu)\,\mathrm{e}^{-S_{\mathrm{YM}}},\; Z_{|\mathrm{QCD}|}=\int\mathcal{D}A\,|\det\gamma_\nu D_\nu|\,\mathrm{e}^{-S_{\mathrm{YM}}}.$$

At $\mu=0$, these two are the same! But,




|QCD| experiences the phase trans. at $\mu=m_\pi/2\sim 70\mathrm{MeV}$.
In QCD, the state = QCD vacuum for $\mu<m_N/3\sim 300\mathrm{MeV}$.

# Complexification of fields

There are two "new" approaches to the sign problem:

- Complex Langevin method: Solve the Langevin eq.

$$\frac{\mathrm{d}z}{\mathrm{d}\theta} = -\frac{\partial S}{\partial z} + \eta(\theta).$$

  $\eta$ is a real stochastic noise, $\langle \eta(\theta)\eta(\theta')\rangle = 2\delta(\theta-\theta')$.
  We have no solid foundations.

- Path integral on Lefschetz thimbles:

$$\int_{\mathbb{R}^n} \mathrm{d}^n x\ \mathrm{e}^{-S(x)} = \sum_{\sigma} \langle \mathcal{K}_\sigma, \mathbb{R}\rangle \int_{\mathcal{J}_\sigma} \mathrm{d}^n z\ \mathrm{e}^{-S(z)}.$$

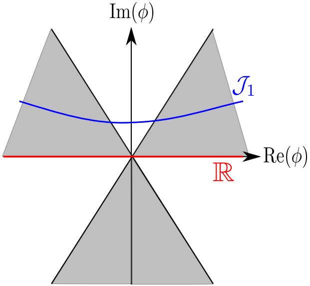
  Path integral is performed on steepest descent paths $\mathcal{J}_\sigma$.
  This is mathematically rigorous.

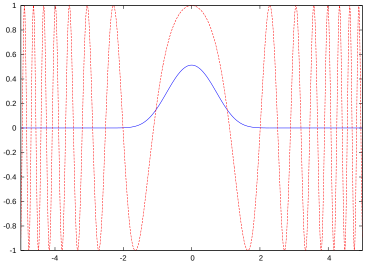
# Lefschetz thimble for Airy integral

Airy integral is given as

$$\mathrm{Ai}(a) = \int_{\mathbb{R}} \frac{\mathrm{d}x}{2\pi} \exp \mathrm{i} \left( \frac{x^3}{3} + ax \right)$$

Complexify the integration variable: $z = x + \mathrm{i}y$.




Integrand on $\mathbb{R}$, and on $\mathcal{J}_1$ $(a = 1)$

# Rewrite the Airy integral

There exists two Lefschetz thimbles $\mathcal{J}_\sigma$ $(\sigma = 1, 2)$ for the Airy integral:

$$\mathrm{Ai}(a) = \sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \frac{\mathrm{d}z}{2\pi} \exp \mathrm{i} \left( \frac{z^3}{3} + az \right).$$

$n_\sigma$: intersection number of the steepest ascent contour $\mathcal{K}_\sigma$ and $\mathbb{R}$.

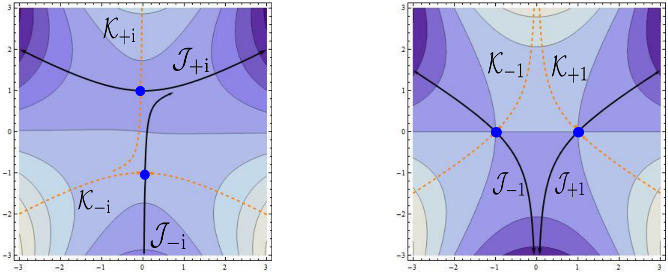



Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ $(a = 1\mathrm{e}^{0.1\mathrm{i}},\ -1)$

# One-site Fermi Hubbard model

One-site Hubbard model:

$$\hat{H} = U\hat{n}_{\uparrow}\hat{n}_{\downarrow} - \mu(\hat{n}_{\uparrow} + \hat{n}_{\downarrow}).$$

Fock state gives the number density immediately:

$$\langle \hat{n} \rangle = \frac{1}{\beta}\frac{\partial}{\partial \mu}\ln Z = \frac{2(\mathrm{e}^{\beta\mu} + \mathrm{e}^{\beta(2\mu-U)})}{1 + 2\mathrm{e}^{\beta\mu} + \mathrm{e}^{\beta(2\mu-U)}}.$$

In the zero-temperature limit,

$$n(\beta=\infty) = \begin{cases} 2 & (1 < \mu/U), \\ 1 & (0 < \mu/U < 1), \\ 0 & (\mu/U < 0). \end{cases}$$

# Path integral for one-site model

The path-integral expression for the one-site Hubbard model: :

$$Z = \sqrt{\frac{\beta}{2\pi U}} \int_{\mathbb{R}} \mathrm{d}\varphi \underbrace{\left(1 + \mathrm{e}^{\beta(\mathrm{i}\varphi + \mu + U/2)}\right)^2}_{\text{Fermion Det}} \mathrm{e}^{-\beta\varphi^2/2U}.$$

Integrand has complex phases causing the sign problem.

$\varphi$ is an auxiliary field for the number density:

$$\langle \hat{n} \rangle = \mathrm{Im}\langle \varphi \rangle / U.$$

# Flows at $\mu/U < -0.5$ and $\mu/U > 1/5$

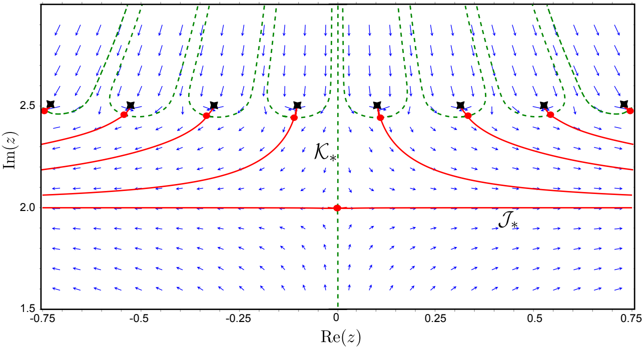



Figure: Flow at $\mu/U = 2$

$$Z = \int_{\mathcal{J}_*} \mathrm{d}z\, \mathrm{e}^{-S(z)}.$$

Number density: $n_* = 0$ for $\mu/U < -0.5$, $n_* = 2$ for $\mu/U > 1.5$.

(YT, Hidaka, Hayata, 1509.07146)

# Flows at $-0.5 < \mu/U < 1.5$

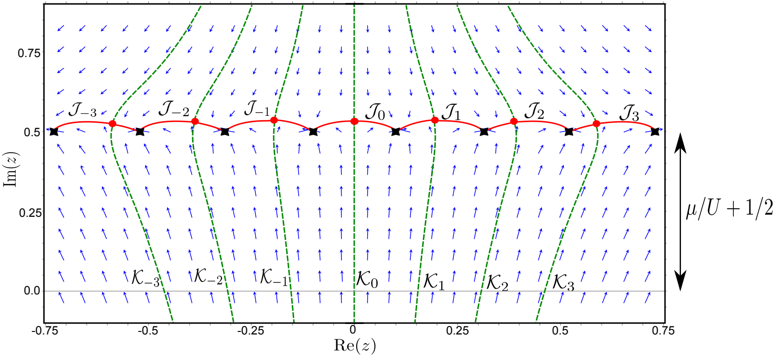



Figure: Flow at $\mu/U = 0$

Complex saddle points lie on $\mathrm{Im}(z_m)/U \simeq \mu/U + 1/2$.

This value is far away from $n = \mathrm{Im}\,\langle z \rangle/U$=0, 1, or 2.

# CL distribution at $-0.5 < \mu/U < 1.5$

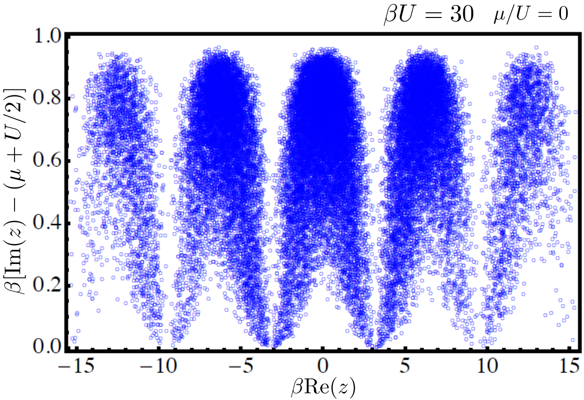
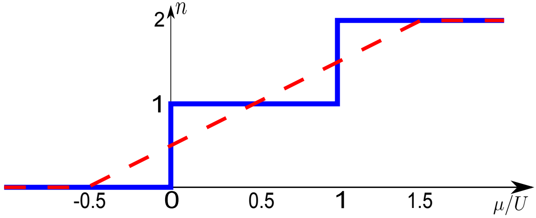



Figure: CL distribution at $\mu/U = 0$

It looks quite similar to Lefschetz thimbles.

# Curious incident of $n$ in the one-site model

We have a big difference bet. the exact result and naive expectation:




CL reproduces the naive one!(YT, Hidaka, Hayata, arXiv:1509.07146, 1511.02437)

This is similar to what happens for QCD and |QCD|.

$\mu/U = -0.5 \Leftrightarrow \mu = m_\pi/2$.

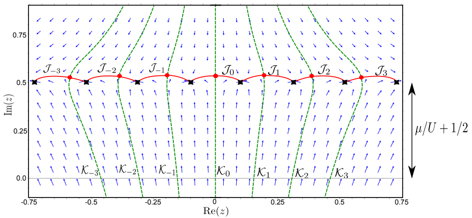
(cf. Monte Carlo with one-thimble approx. gives the naively expected results.

Fujii, Kamata, Kikukawa,1509.08176, 1509.09141; Alexandru, Basar, Bedaque,1510.03258)

# Complex classical solutions

If $\beta U \gg 1$, the classical sol. for $-0.5 < \mu/U < 1.5$ are labeled by $m \in \mathbb{Z}$:

$$z_m \simeq \mathrm{i}\left(\mu + \frac{U}{2}\right) + 2\pi m T.$$




At these solutions, the classical actions become

$$S_0 \simeq -\frac{\beta U}{2}\left(\frac{\mu}{U}+\frac{1}{2}\right)^2,$$

$$\mathrm{Re}\left(S_m - S_0\right) \simeq \frac{2\pi^2}{\beta U} m^2,$$

$$\mathrm{Im}\, S_m \simeq 2\pi m \left(\frac{\mu}{U}+\frac{1}{2}\right).$$

# Semiclassical partition function

Using complex classical solutions $z_m$, let us calculate

$$Z_{\rm cl} := \sum_{m=-\infty}^{\infty} \mathrm{e}^{-S_m}.$$

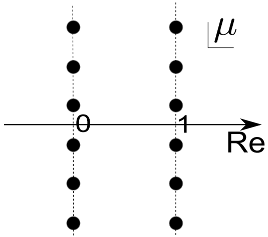
This expression is valid for $-1/2 \lesssim \mu/U \lesssim 3/2$.

This is calculable using the elliptic theta function:

$$\begin{aligned} Z_{\rm cl} &\simeq \mathrm{e}^{-S_0}\left(1+2\sum_{m=1}^{\infty} \cos 2\pi m \left(\frac{\mu}{U}+\frac{1}{2}\right) \mathrm{e}^{-2\pi^2 m^2/\beta U}\right) \\ &= \mathrm{e}^{-S_0}\theta_3\left(\pi\left(\frac{\mu}{U}+\frac{1}{2}\right), \mathrm{e}^{-2\pi^2/\beta U}\right). \end{aligned}$$

# Number density & Lee–Yang zeros

Lee–Yang zeros of $Z_{\rm cl}$:




Semiclassical study gives the correct transition!

$$n_{\rm cl} := \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z_{\rm cl} \to \begin{cases} 2 & (1<\mu/U<3/2), \\ 1 & (0<\mu/U<1), \\ 0 & (-1/2<\mu/U<0). \end{cases}$$

(YT, Hidaka, Hayata, arXiv:1509.07146[hep-th])

# Important interference among multiple thimbles

Let us consider a "phase-quenched" multi-thimble approximation:

$$Z_{|\mathrm{cl.}|} = \sum_m \left|\mathrm{e}^{-S_m}\right| = \mathrm{e}^{-S_0(\mu)}\theta_3(0, \mathrm{e}^{-2\pi^2/\beta U}).$$

- Lee–Yang zeros cannot appear at $\mu/U = 0,\, 1$.
- One-thimble, or "phase-quenched", result: $n \simeq \mu/U + 1/2$.
- Complex Langevin $\simeq$ the phase-quenched multi-thimble approx.

## Consequence

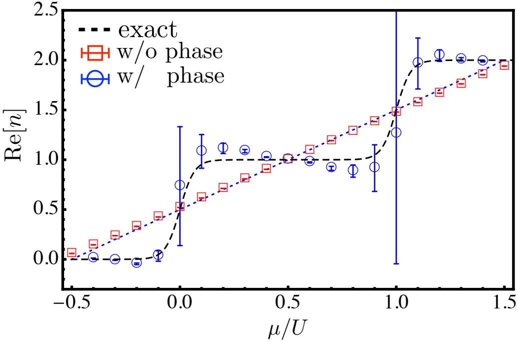
*In order to describe the step functions, we need interference of complex phases among different Lefschetz thimbles.*

(cf. Particle Productions: Dumulu, Dunne, PRL 104 250402)

(cf. Hidden Topological Angles: Behtash, Sulejmanpasic, Schäfer, Ünsal, PRL 115 041601)

# Complex Langevin simulation

One-site Fermi Hubbard model:




(Hayata, Hidaka, YT, arXiv:1511.02437[hep-lat])

## Consequence

*Modified complex Langevin is not perfect yet, but it seems to point a correct way. I hope this can attack the Silver Blaze phenomenon.*

# Summary and Conclusion

- Picard–Lefschetz theory gives a suitable framework for saddle-point analysis even if $S(\phi)$ takes complex values.
- One-site Hubbard model is a nice toy model to play with the sign problem.
- Destructive and constructive interference of complex phases among Lefschetz thimbles play a pivotal role for the baryon Silver Blaze.

# Backups

# Lefschetz decomposition formula

Oscillatory integrals with **many variables** can be evaluated using the "steepest descent" cycles $\mathcal{J}_\sigma$: (classical eom $S'(z_\sigma)=0$)

$$\int_{\mathbb{R}^n} \mathrm{d}^n x\, \mathrm{e}^{-S(x)} = \sum_\sigma \langle \mathcal{K}_\sigma, \mathbb{R}\rangle \int_{\mathcal{J}_\sigma} \mathrm{d}^n z\, \mathrm{e}^{-S(z)}.$$

$\mathcal{J}_\sigma$ are called Lefschetz thimbles, and $\mathrm{Im}[S]$ is constant on it:

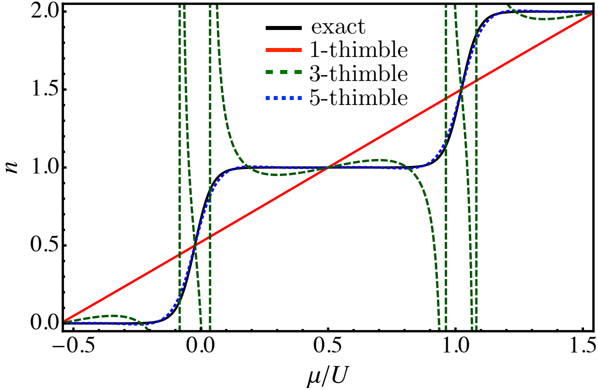
$$\mathcal{J}_\sigma = \left\{ z(0) \middle| \lim_{t\to-\infty} z(t) = z_\sigma \right\}, \quad \frac{\mathrm{d}z^i(t)}{\mathrm{d}t} = \overline{\left(\frac{\partial S(z)}{\partial z^i}\right)}.$$

$\langle \mathcal{K}_\sigma, \mathbb{R}\rangle$: intersection numbers of duals $\mathcal{K}_\sigma$ and $\mathbb{R}^n$
($\mathcal{K}_\sigma = \{z(0) | z(\infty) = z_\sigma\}$).

[Witten, arXiv:1001.2933, 1009.6032]

# Numerical results

Results for $\beta U = 30$: (1, 3, 5-thimble approx.: $\mathcal{J}_0$, $\mathcal{J}_0 \cup \mathcal{J}_{\pm 1}$, and $\mathcal{J}_0 \cup \mathcal{J}_{\pm 1} \cup \mathcal{J}_{\pm 2}$ )




(YT, Hidaka, Hayata, arXiv:1509.07146[hep-th])

# Complex Langevin method

Complex Langevin has been regarded as a sign-problem solver via stochastic quantization (Klauder, PRA 29, 2036 (1984), Parisi, PLB 131, 393 (1983)):

$$\frac{\mathrm{d}z_\eta(\theta)}{\mathrm{d}\theta}=-\frac{\partial S}{\partial z}(z_\eta(\theta))+\sqrt{\hbar}\eta(\theta).$$

$\theta$: Stochastic time, $\eta$: Random force satisfying $\langle\eta(\theta)\eta(\theta')\rangle_\eta=2\delta(\theta-\theta')$.

Itô calculus shows that

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\langle O(z_\eta(\theta))\rangle_\eta=\hbar\langle O''(z_\eta(\theta))\rangle_\eta-\langle O'(z_\eta(\theta))S'(z_\eta(\theta))\rangle_\eta.$$

If the l.h.s becomes zero as $\theta\to\infty$, this is nothing but the Dyson–Schwinger eq.

# Complex Langevin and Lefschetz thimbles

For any solutions of the DS eq,

$$\langle O(z_\eta)\rangle_\eta = \frac{1}{Z}\sum_\sigma {}^\exists d_\sigma \int_{\mathcal{J}_\sigma} \mathrm{d}z\, \mathrm{e}^{-S(z)/\hbar} O(z),$$

in $d_\sigma \in \mathbb{C}$. To reproduce physics, $d_\sigma = \langle \mathcal{K}_\sigma, \mathbb{R}\rangle$.

So far, we ONLY assume the convergence of the complex Langevin method.

# Semiclassical limit

Let us take $\hbar \ll 1$ for computing

$$\langle O(z_\eta)\rangle_\eta = \frac{1}{Z}\sum_\sigma d_\sigma \int_{\mathcal{J}_\sigma} \mathrm{d}z\, \mathrm{e}^{-S(z)/\hbar} O(z).$$

I have NO idea how to compute the LHS. However, positivity of the probability density and its localization around $z_\sigma$'s imply that

$$^\exists c_\sigma \geq 0 \quad \text{s.t.} \quad \langle O(z_\eta)\rangle_\eta \simeq \sum_\sigma c_\sigma O(z_\sigma).$$

RHS is

$$\int_{\mathcal{J}_\sigma} \mathrm{d}z\, \mathrm{e}^{-S(z)/\hbar} O(z) \simeq \sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}} \mathrm{e}^{-S(z_\sigma)/\hbar} O(z_\sigma).$$

# Semiclassical inconsistency

In the semiclassical analysis, one obtains (for dominant saddle points)

$$c_\sigma = \frac{d_\sigma}{Z}\sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}}\mathrm{e}^{-S(z_\sigma)/\hbar}.$$

$c_\sigma \geq 0$. And, $d_\sigma = \langle K_\sigma, \mathbb{R}\rangle$ to get physics. $\Rightarrow$ Inconsistent!

(Hayata, Hidaka, YT, arXiv:1511.02437[hep-lat])

We show that the complex Langevin is wrong if

- There exist several dominantly contributing saddle points.
- Those saddle points have different complex phases.

**Consequence**

*Naive complex Langevin method cannot explain the Silver Blaze phenomenon.*

# Proposal for modification

Assume that

$$c_\sigma = \frac{\langle \mathcal{K}_\sigma, \mathbb{R}\rangle}{Z}\left|\sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}}\mathrm{e}^{-S(z_\sigma)/\hbar}\right|.$$

Because of the localization of probability distribution $P$, it would be given as

$$P = \sum_\sigma c_\sigma P_\sigma, \quad \mathrm{supp}(P_\sigma) \cap \mathrm{supp}(P_\tau) = \emptyset.$$

Assumption means "CL = phase quenched multi-thimble approx.":

$$\langle O(z_\eta)\rangle_\eta \simeq \sum_\sigma \frac{\langle \mathcal{K}_\sigma, \mathbb{R}\rangle}{Z}\left|\sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}}\mathrm{e}^{-S(z_\sigma)/\hbar}\right| O(z_\sigma).$$

# Proposal for modification (conti.)

If so, defining the phase function

$$\Phi(z,\overline{z}) = \sum_\sigma \sqrt{\frac{|S''(z_\sigma)|}{S''(z_\sigma)}} \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}\,S(z_\sigma)/\hbar} \chi_{\mathrm{supp}(\mathrm{P}_\sigma)}(z,\overline{z}),$$

we can compute

$$\langle O(z_\eta)\rangle^{\mathrm{new}} := \frac{\langle \Phi(z_\eta,\overline{z}_\eta) O(z_\eta)\rangle_\eta}{\langle \Phi(z_\eta,\overline{z}_\eta)\rangle_\eta}.$$

This new one is now consistent within the semiclassical analysis.

(Hayata, Hidaka, YT, arXiv:1511.02437[hep-lat])